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Hybridized Multiscale Discontinuous Galerkin Methods for Multiphysics

Jaime Peraire
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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We have continued the development of the Hybridized Discontinuous Galerkin (HDG) method for the solution of systems of conservation laws. The focus has been on the development of robust, accurate, and efficient methods capable of handling complex physics in realistic geometries. In particular, we have: 1) proposed a Hybridized Multiscale Discontinuous Galerkin method (HMDG), 2) extended the HDG approximation to second-order elliptic eigenvalue problems, 3) presented a new phased-based method for high frequency wave propagation, 4) presented an embedded discontinuous Galerkin (EDG) method , 5) introduced a novel shock capturing technique, and 6) presented a novel approach for UQ

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HYBRIDIZED DISCONTINUOUS GALERKIN METHODS FOR MULTIPHYSICS

J. Peraire and C. N. Nguyen

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Title: Hybridizable Discontinuous Galerkin (HDG) Methods for Systems of Conservation Laws

In recent years, discontinuous Galerkin (DG) methods have attracted considerable attention because they possess a number of desirable properties for solving hyperbolic systems of conservation laws. In particular, the DG methods work well on arbitrary meshes, result in stable high-order discretization of the convective and diffusive operators, allow for a simple and unambiguous imposition of boundary conditions, and are well-suited to adaptive strategies. However, the DG methods have been criticized for providing sub-optimally convergent approximations for the flux, as well as for producing a substantially larger amount of globally-coupled degrees of freedom (for the same mesh and polynomial degree of the approximation) in comparison to the well-established finite element methods for diffusion problems. In response to these criticisms, the hybridizable discontinuous Galerkin (HDG) methods were first introduced in [1] and later extended in [2], [3], [4], [5], [6], [7], [8], [9]. The essential ingredients are a local Galerkin projection of the underlying PDEs at the element level onto spaces of polynomials of degree k to parametrize the numerical solution in terms of the numerical trace; a judicious choice of the numerical flux to provide stability and consistency; and a global jump condition that enforces the continuity of the numerical flux to arrive at a global weak formulation in terms of the numerical trace. The HDG method is fully implicit, high-order accurate and endowed with several unique features which distinguish themselves from other discontinuous Galerkin methods. First, they reduce the globally coupled unknowns to the approximate trace of the solution on element boundaries, thereby leading to a significant reduction in the degrees of freedom. Second, they provide, for smooth viscous-dominated problems, approximations of all the variables which converge with the optimal order of $k + 1$ in the L_2-norm. Third, they possess some superconvergence properties that allow us to define inexpensive element-by-element postprocessing procedures to compute a new approximate solution which may converge with higher order than the original solution. And fourth, they allow for a novel and systematic way for imposing boundary conditions for the total stress, viscous stress, vorticity, and pressure which are not naturally associated with the weak formulation of the methods. In addition, they possess other interesting properties for specific problems. Their approximate solution can be postprocessed to yield an exactly divergence-free and $H(\mathrm{div})$-conforming velocity field for incompressible flows. They do not exhibit volumetric locking for nearly incompressible solids.

The first HDG method for the compressible Euler and Navier-Stokes equations was introduced in [10]. This method possesses a number of desirable properties. First, in implicit formulations, it reduces the globally coupled unknowns to the numerical trace of the solution on element boundaries, thereby leading to a significant reduction in the degrees of freedom. Second, it provides, for smooth (e.g., viscous-dominated) problems, approximations for all the variables which converge with the optimal order of $k + 1$ in the L^2-norm. Third, it possesses superconvergence properties that allow us to compute a new approximate velocity which converges with order $k+2$ for $k \geq 1$. And fourth, it allows for a novel and systematic way

for imposing general (external or internal) boundary conditions.

In this grant, we have continued the development of Hybridized Discontinuous Galerkin (HDG) methods for the solution of systems of conservation laws. In particular, the focus has been the development of robust, accurate, and efficient methods capable of handling complex physics in realistic geometries. Below, we describe the main research results.

I. Research Results

A. Multiscale HDG Method

We have introduced a hybridized multiscale discontinuous Galerkin (HMDG) method for the numerical solution of compressible flows [11]. The HMDG method is developed upon extending the hybridizable discontinuous Galerkin (HDG) by modifying the local approximation spaces on elements. The essential ingredients are (1) a local Galerkin projection of the underlying PDEs at the element level onto suitable local approximation spaces, (2) a judicious choice of the numerical flux to provide stability and consistency, and (3) a global jump condition that enforces the continuity of the numerical flux to arrive at a global system in terms of the numerical trace. The local approximation spaces are characterized by two integers (n^*, k^*), where $n^* \in [1, n]$ is the number of subcells within an element and $k^* \in [0, k]$ is the polynomial degree of shape functions defined on the subcells. The selection of the value of (n^*, k^*) on a particular element depends on the smoothness of the solution on that element. More specifically, for elements on which the solution is smooth, we choose the smallest value $n^* = 1$ and the highest degree $k^* = k$. For elements containing shocks in the solution, we use the largest value $n^* = n$ and the lowest degree $k^* = 0$. The proposed method thus combines the accuracy and efficiency of high-order approximations with the robustness of low-order approximations. A key advantage of the HMDG method is that it can capture shocks without using artificial viscosity and limiting slopes/fluxes.

B. Eigenvalue Problems

We have introduced hybridization and postprocessing techniques for the HDG approximation of second-order elliptic eigenvalue problems [12]. Hybridization reduces the HDG approximation to a condensed eigenproblem. The condensed eigenproblem is nonlinear, but smaller than the original mixed approximation. We derived iterative algorithms for solving the condensed eigenproblem and examined their interrelationships and convergence rates. For smooth eigenfunctions, the approximate eigenvalues and eigenfunctions converge at the rate $2k + 1$ and $k + 1$, respectively. Here k is the degree of the polynomials used to approximate the solution, its flux, and the numerical traces. An element-by-element postprocessing technique to improve accuracy of computed eigenfunctions is also presented. We prove that a projection of the error in the eigenspace approximation superconverges and that the postprocessed eigenfunction approximations converge faster for smooth eigenfunctions. Our numerical studies showed that a Rayleigh quotient-like formula applied to the locally postprocessed approximations can yield eigenvalues that converge faster at the rate $2k + 2$

C. Phased-based Methods for Wave Propagation

For wave propagation [13], we have presented a new class of HDG methods capable of generating high-quality approximations of the Helmholtz equation for a very wide range of wave frequencies. Our approach combines the hybridizable discontinuous Galerkin methodology with the geometrical optics in an elegant fashion that allows us to take advantage of the strengths of these two methodologies. First, we enrich the local approximation spaces of the hybridizable discontinuous Galerkin methods with precomputed phases which are solutions of the eikonal equation in geometrical optics. Second, we propose a systematic procedure for computing multiple solutions of the eikonal equation. Third, we utilize the eigenvalue decomposition to remove redundant modes and obtain orthogonal basis functions. And fourth, these locally

orthogonal approximation spaces are used to define the global approximation spaces of the phase-based HDG methods. This class of methods possesses a number of critical advantages over the current state-of-the-art low-frequency and high-frequency schemes. Unlike other numerical methods which require the degrees of freedom to increase drastically with the wave number, the proposed methods can provide full-wave solutions with a fixed number of degrees of freedom for a wide range of frequencies. Unlike asymptotic high-frequency methods which may not be rigorous and accurate for moderate frequencies, they provide accurate and reliable approximations for moderate frequencies. We present several numerical examples to demonstrate the performance of the proposed approach.

D. Embedded Discontinuous Galerkin Methods (EDG)

We have presented an embedded discontinuous Galerkin (EDG) method for numerically solving the Euler equations and the Navier-Stokes equations [14]. The essential ingredients are a local Galerkin projection of the underlying governing equations at the element level onto spaces of polynomials of degree k to parametrize the numerical solution in terms of the approximate trace, a judicious choice of the numerical flux to provide stability and consistency, and a global jump condition that weakly enforces the single-valuedness of the numerical flux to arrive at a global formulation in terms of the numerical trace. The EDG method is thus obtained from a Hybridizable Discontinuous Galerkin (HDG) method by requiring the approximate trace to belong to a smaller space than the one in the HDG method. In the EDG method, the numerical trace is taken to be continuous, thus resulting in an even smaller number of globally coupled degrees of freedom than in the HDG method. On the other hand, the EDG method is no longer locally conservative. In the framework of convection-diffusion problems, this lack of local conservativity is reflected in the fact that the EDG method does not provide the optimal convergence of the approximate gradient or the superconvergence for the scalar variable for diffusion-dominated problems as the HDG method does. However, since the HDG method does not display these properties in the convection-dominated regime, the associated EDG method becomes a reasonable alternative since it produces smaller algebraic systems than the HDG method. In fact, the resulting stiffness matrix has the same sparsity structure as that of the statically condensed continuous Galerkin (CG) method. The main advantage of the EDG method is that it is more stable and robust than the CG method for solving convection-dominated problems. Numerical results indicate that, even though the EDG method is not locally conservative, it is a viable alternative to the HDG method in the convection-dominated regime.

E. Shock Capturing

We have introduced a novel shock capturing artificial viscosity technique [15] for high-order unstructured mesh methods. This artificial viscosity model is based on a non-dimensional form of the divergence of the velocity. The approach presented has a number of attractive properties, over previously presented methods, including non-dimensional analytical form, sub-cell resolution, and robustness for complex shock flows on highly anisotropic meshes. We presented extensive numerical results to demonstrate the performance of the proposed approach.

F. Explicit HDG

We have presented an explicit hybridizable discontinuous Galerkin (HDG) method for the acoustic wave equation [16]. The method provides optimal convergence of order $k+1$ for all the approximate variables including the gradient of the solution, and, when the time-stepping method is of order $k+2$, it displays a superconvergence property which allow us, by means of local post-processing, to obtain new improved approximations of the scalar field variables at any time level. In particular, the new approximations converge with order $k+2$ in the L_2-norm for k equal to 1 or greater. These properties do not hold for all numerical fluxes. Indeed, our results show that, when the HDG numerical flux is replaced by the Lax-Friedrichs flux, the above-mentioned super-convergence properties are lost.

G. Electromagnetics: An Application in Nanophotonics

We have used our HDG method to solve Maxwell's equations for a nanophotonics application [17]. First, we experimentally show that terahertz (THz) waves confined in sub-10 nm metallic gaps can detect refractive index changes caused by only a 1 nm thick $(\sim \lambda/106)$ dielectric overlayer. We use atomic layer lithography to fabricate a wafer-scale array of annular nanogaps. Using THz time-domain spectroscopy in conjunction with atomic layer deposition, we measure spectral shifts of a THz resonance peak with increasing Al_2O_3 film thickness in 1 nm intervals. Because of the enormous mismatch in length scales between THz waves and sub-10 nm gaps, conventional modeling techniques cannot readily be used to analyze our results. We employ our Hybridizable Discontinuous Galerkin (HDG) scheme, for full three-dimensional modeling of the resonant transmission of THz waves through an annular gap that is 2 nm in width and 32 μm in diameter. Our multiscale 3D FEM technique and atomic layer lithography will enable a series of new investigations in THz nanophotonics that has not been possible before.

H. Uncertainty Quantification

In the last year of the grant, we have presented a new statistical approach to the problem of incorporating experimental observations into a mathematical model described by linear partial differential equations (PDEs) to improve the prediction of the state of a physical system [18]. We augment the linear PDE with a functional that accounts for the uncertainty in the mathematical model and is modeled as a Gaussian process. We develop a Gaussian functional regression method to determine the posterior mean and covariance of the Gaussian functional, thereby solving the stochastic PDE to obtain the posterior distribution for our prediction of the physical state. Our method has the following features which distinguish itself from other regression methods. First, it incorporates both the mathematical model and the observations into the regression procedure. Second, it can handle the observations given in the form of linear functionals of the field variable. Third, the method is non-parametric in the sense that it provides a systematic way to optimally determine the prior covariance operator of the Gaussian functional based on the observations. Fourth, it provides the posterior distribution quantifying the magnitude of uncertainty in our prediction of the physical state. In [19], we built on the previous work but considered the problem of experimental design. We developed an algorithm for designing experiments to efficiently reduce the variance of our state estimate. We provide several examples from heat conduction, the convection-diffusion equation, and the reduced wave equation, all of which demonstrate the performance of the proposed methodology. Finally, in [20] we introduced a Gaussian functional regression (GFR) technique that integrates multi-fidelity models with model reduction to efficiently predict the input-output relationship of a high-fidelity model. We developed a greedy sampling algorithm to select the training inputs. Our approach results in an output prediction model that inherits the fidelity of the high-fidelity model and has the computational complexity of the reduced basis approximation.

We expect to continue this line of research in the future.

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Primary Contat Phone Number:	617-253-1981
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	capturing artificial viscosity technique for high-order unstructured mesh methods, 6) introduced an explicit hybridizable discontinuous Galerkin (HDG) method for the acoustic wave equation, and finally, 7) presented a new statistical approach to the problem of incorporating experimental observations into a mathematical model described by linear partial differential equations (PDEs) to improve the prediction of the state of a physical system. We have also illustrated our methods on number of applications in fluid mechanics and electromagnetics.
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